Three-dimensionally periodic dielectric layered structure with omnidirectional photonic band gap

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A three-dimensionally periodic dielectric structure with a large complete photonic band gap (PBG) is presented. The structure is distinguished by a sequence of planar layers, identical except for a horizontal offset, and repeating every three layers to form an fcc lattice. The layers can be thought of as an alternating stack of the two basic two-dimensional (2D) PBG slab geometries: rods in air and air cylinders in dielectric. These high-symmetry planar cross-sections should simplify the integration of optical devices and components by allowing modification of only a single layer, using simple defects of the same form as in the corresponding 2D systems. A process for fabricating the structure with conventional planar microfabrication technology is described. Gaps of over 21% are obtained for Si/air substrates. Reasonable gaps, over 8%, can be achieved even for the moderate index ratio of 2.45 (Si/SiO_2). © *2000 American Institute of Physics.* [S0003-6951(00)00848-2]

Much research in recent years has been focused on photonic crystals—periodic dielectric (or metallic) structures with a photonic band gap (PBG), a range of frequencies in which light is forbidden to propagate.[1,2] Photonic crystals provide an unprecedented degree of control over light, introducing the possibility of many novel optical devices and effects.[3] The diamond, A7, and graphite geometries have been shown to be particularly promising for PBGs, and these have led to many interesting practical structures.[4–13] We present a design (depicted in Fig. 1) for a practical three-dimensional photonic crystal based on these geometries. Our design satisfies three desirable criteria: (i) it has a large, complete PBG; (ii) it is a stack of planar layers amenable to microfabrication; and (iii) each layer corresponds to one of the two basic, ubiquitous two-dimensional (2D) photonic-crystal slab geometries: rods in air and air cylinders in dielectric. The third criterion distinguishes our structure from previous work, and the resulting high-symmetry cross sections should allow integrated optical networks to be formed by changing only a *single* layer. In this way, one can leverage the extensive analyses and results obtained for 2D slab structures,[14] without incurring the intrinsic losses due to the lack of an omnidirectional gap.

The structure we propose is simply an fcc lattice (possibly distorted) of air (or low-index) cylinders in dielectric, oriented along the 111 direction. Such a structure, depicted in Fig. 1, results in a graphitelike[5] system of planar ''slabs'' (two-dimensionally periodic, finite height) of two types: triangular lattices of air holes in dielectric and dielectric cylinders (''rods'') in air. The sculptured appearance of the rods is not important and is simply a by-product of the fabrication method (in Fig. 2). These slabs are stacked in a repeating, three-layer sequence (along 111) and should be amenable to planar lithographic techniques as described in the following. The band diagram, in Fig. 3(a), has a complete gap of over 21% for Si:air dielectric contrast ($\epsilon=12:1$ at 1.55 μm), and of over 8% even for $Si:SiO_2$ contrast ($\epsilon=12:2$); the PBG persists down to ϵ contrasts of 4:1 (2:1 index contrast). The vertical transmission through roughly one period (three layers plus a hole slab) of the structure, shown in Fig. 3(b), is attenuated by about 20 dB in the gap.

Considered individually, such ''photonic-crystal slab'' layers have been the subject of much recent study,[14] because they form a convenient and easily fabricated approximation to two-dimensional photonic crystals. By themselves, however, they do not have a complete PBG and rely on index guiding for vertical confinement, with consequential radiation losses whenever translational symmetry is broken (e.g., at a waveguide bend or resonant cavity). Our structure overcomes this difficulty, and retains the advantage of a highly symmetric cross section—a ''2D photonic crystal'' in three dimensions. In the same system, one may then effectively work with either ''rod'' or ''hole'' 2D crystals, with the analogous characters of the modes and defects (e.g., waveguides and cavities).

The ideal photonic crystal structure is one with an omnidirectional band gap in three dimensions, and can thus be used to control light without losses regardless of propagation direction. A large gap (measured as a percentage of midgap frequency) is desirable because it displays the biggest optical effects, has the strongest confinement (allowing smaller crystals and devices), is robust in the presence of experimental disorder, and allows the widest bandwidth for optical devices. Most structures with complete PBGs are described by a diamond structure[4] or fcc lattice, or a distorted cousin such as an A7 or graphite structure,[5] due to their ''near-spherical'' Brillouin zones. Although this determines the underlying topology and periodicity of the geometry, substantial innovations were required in order to design practically realizable structures at micron length scales. One class of systems, typified by the ''inverse opal''[6–8] (an fcc lattice of air spheres in dielectric), is constructed by self-assembly or similar methods—this can have unique advantages (e.g., inexpensive large-scale growth), but typically lacks the fine control pro-

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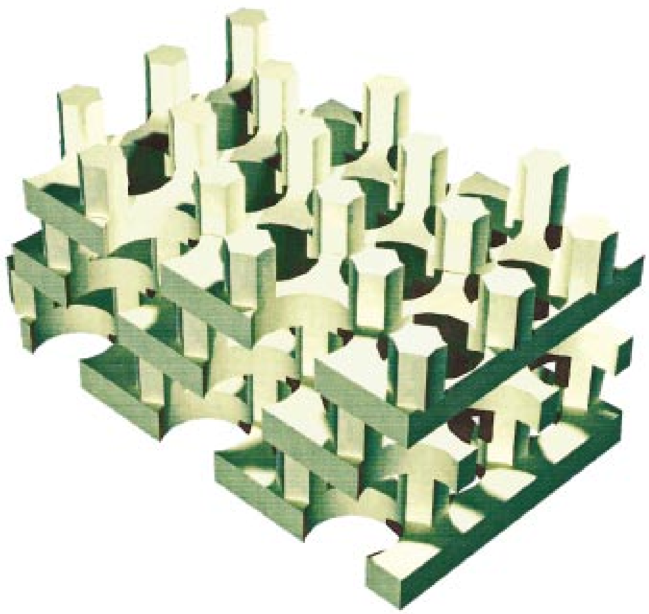

FIG. 1. (Color) Computer rendering of a novel 3D photonic crystal, showing several horizontal periods and one vertical period, consisting of an fcc lattice of air holes (radius 0.293a, height 0.93a) in dielectric (21% fill). This structure has a 21% gap for a dielectric constant of 12.

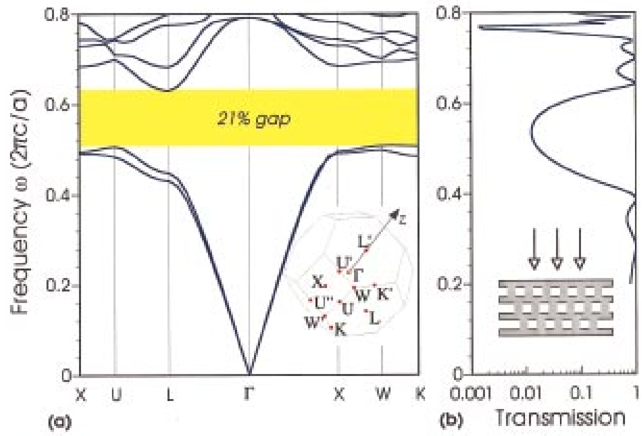

FIG. 3. (Color) (a) Band diagram for the structure in Fig. 1, showing frequency in scale-invariant units vs wave vector along important symmetry directions in the irreducible Brillouin zone. The inset shows the first Brillouin zone and its symmetry points. (b) Vertical transmission spectrum for slightly over one period (three layers plus a capping hole slab, as shown in the inset) of this structure, showing the $\Gamma-L'$ gap.

vided by direct etching. Another PBG design, based on the diamond structure, is an fcc lattice oriented vertically in the 111 direction and formed by drilling a set of angled holes (along 110) into a bulk material.[9] A third class of designs, including ours, consists of planar layers with piecewise-constant cross sections, which can be fabricated layer by layer—this provides the ability to place defects and devices in the lattice with very fine control. An often-fabricated planar-layer structure is the ''layer-by-layer''[10] (or ''woodpile''[11]) design: dielectric ''logs'' stacked in alternating perpendicular directions with a four-layer period, forming an fcc crystal oriented in the 100 direction. Any given plane, however, does not have high rotational symmetry, meaning that complicated optical systems (with symmetric waveguides in various directions) must be formed by modifying at least two layers. A similar structure with more complicated logs (to more closely mimic a diamond structure) has also been proposed.[12] An entirely different planar-layer three-dimensional (3D) PBG was designed using an fcc lattice stacked in the 110 direction,[13] with a 23% gap for $\epsilon=12:1$—however, it lacks planar rotational symmetry, prohibiting identical waveguides along different directions (desirable for integrated optics). There is one planar-layer PBG structure with a complete gap that does have highly symmetric cross sections—the simple-cubic ''scaffold'' lattice[15] with square rods along the edges of the cubes. (This is the exception to the rule of fcc-like lattices.) In a sense, this structure is similar to the one we propose, albeit in a simple-cubic rather than fcc lattice—it consists of alternating layers of thin slabs of square holes and thick slabs of square rods. The maximum gap achievable in the cubic scaffold for $\epsilon=12:1$ is 7%.

The band diagram depicted in Fig. 3(a) is for air holes of radius $r=0.293a$ and height $h=0.93a$ (a is the fcc lattice constant) and a dielectric constant $\epsilon=12$, and has a 20.9% complete PBG. The bands were computed using preconditioned conjugate-gradient minimization of the Rayleigh quotient in a plane-wave basis.[16,17] (There are other symmetry points in the irreducible Brillouin zone of this structure that were calculated but are not shown in the band diagram, because their band edges do not determine the gap in this case.) The transmission spectrum of Fig. 3(b) is the result of a 3D finite-difference time-domain simulation[18] with a normal-incidence ($\Gamma-L'$) plane-wave source, absorbing boundaries above and below, and periodic boundaries at the sides.

More generally, one can apply a trigonal distortion to the fcc lattice of our structure to obtain a trigonal lattice without breaking any additional symmetry. The lattice vectors in this

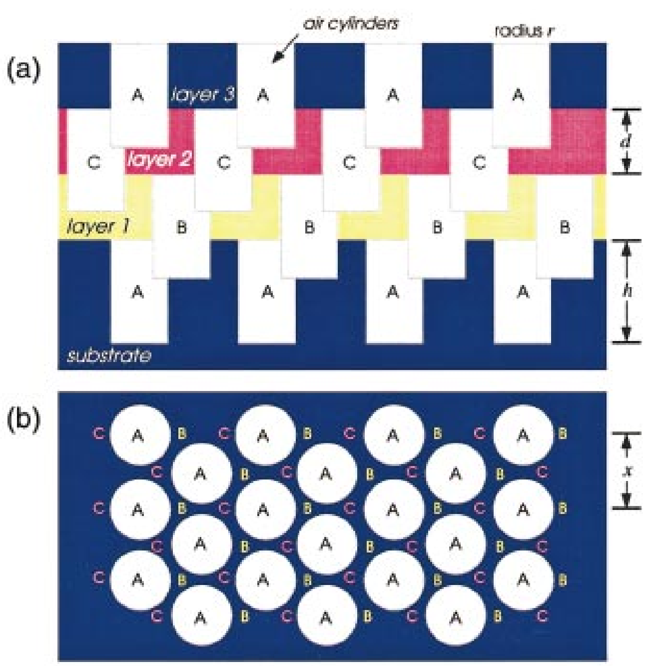

FIG. 2. (Color) Schematic of the crystal in Fig. 1. (a) The vertical structure, showing the different material layers as they might be deposited during fabrication. (The layers are given different colors for clarity, but would normally be the same material and thickness.) (b) Plan view of a horizontal cross section intersecting the ''A'' cylinders, with the offset locations of cylinders in other layers also labeled.

TABLE I. Optimal parameters and gaps for various dielectric constants.

ϵ contrast	r	h	z	Midgap ν	Gap size
12:1 (Si:air)	$0.285a$	$0.960a$	0.016 5	0.579 c/a	21.4%
6:1	$0.273a$	$0.908a$	−0.002 46	0.648 c/a	8.4%
12:2 (Si/SiO_2)				0.458 c/a	
4.5:1	$0.265a$	$0.900a$	−0.006 12	0.688 c/a	2.7%
4:1 (SiO_2:air)	$0.259a$	$0.895a$	−0.007 78	0.699 c/a	0.33%

case become the three permutations of $(a/2)(1,1,z)$ $(z=0$ for fcc), with

$$d=\frac{a}{\sqrt{3}}\left|1+\frac{z}{2}\right|$$

and

$$x=\frac{a}{\sqrt{2}}|1-z|$$

as defined in Fig. 2. The parameter z can be varied to optimize the gap. The parameters of Fig. 3 were optimal for the fcc case of $z=0$; we also maximized the gap for varying z and dielectric contrast, with results in Table I. In general, the structure strongly prefers the fcc case with its nearly spherical Brillouin zone, and distortion seems to increase the gap percentage by no more than 0.5.

The fabrication of our structure might proceed along the following schematic lines, as depicted in Fig. 2. First, a layer of cylindrical holes (labeled ''A'') is etched into a high-index substrate (e.g., Si). Next, the holes are backfilled with another material (e.g., SiO_2), the surface is planarized to the top of the high-index substrate, and a second layer of high-index material (''layer 1'') is grown on top. Then, the next layer of holes (''B'') is etched to the appropriate depth, but offset from the ''A'' holes as shown in Fig. 2(b). This backfilling, planarizing, growth, and etching is repeated for the ''C'' holes and then for the next layer of ''A'' (in ''layer 3''), at which point the structure repeats itself. When the desired layers are grown, the backfill material is removed (e.g., by a solvent), and a high-contrast photonic crystal is obtained. A similar process has been successfully employed for the ''layer-by-layer'' structure, testifying to the feasibility of this method.[19,20] Other variations are possible. One could leave the backfill material in the structure if it is low index, and a complete PBG (albeit smaller, 8.4% for Si/SiO_2) can still be obtained; equivalently, a lower-index substrate could be used with air holes. Also, the layers could be fabricated individually, and then inverted and bonded together; this method has likewise been proven on the layer-by-layer structure.[21,22] Alternatively, one may fabricate the rod and hole slabs using separate steps, requiring twice as many interlayer alignments but removing the need to etch two materials simultaneously. (It has recently come to our attention that a very similar structure was thus fabricated for 8 μm wavelength, although the existence of a gap was not determined.[23]) Our calculations show that the resulting extra degree of freedom, the rod radius, allows a maximum gap of over 26% for Si/air.

In summary, we have demonstrated a photonic crystal structure with a complete three-dimensional band gap. This structure has a very large gap, is tolerant of low index contrast, is amenable to layer-by-layer fabrication, and can be thought of as a stack of 2D photonic-crystal slabs. This last feature, in the context of a large three-dimensional gap, permits simplified construction of complicated optical networks by modifying only a single layer, without breaking symmetry between different directions in the plane. The defect modes thus created are expected to have much of the simple, well-understood character of the modes in the analogous 2D photonic crystals/slabs (both rod and hole lattices)—thereby building on the large body of existing work and analyses for those basic systems, without the inherent problems of losses due to the lack of a complete PBG.

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